



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 07:11 PM UTC

PDB ID : 3MBE / pdb_00003mbe
Title : TCR 21.30 in complex with MHC class II I-Ag7HEL(11-27)
Authors : Corper, A.L.; Yoshida, K.; Teyton, L.; Wilson, I.A.
Deposited on : 2010-03-25
Resolution : 2.89 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

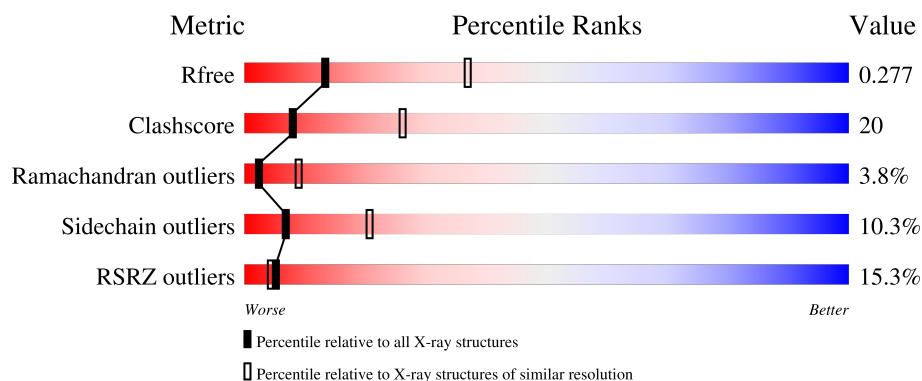
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	190	6% 59% 32% 5% • •
1	E	190	21% 58% 34% • • •
2	B	201	6% 50% 30% 8% 11%
2	F	201	20% 50% 30% 8% 11%
3	P	18	11% 44% 33% 17% 6%

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Mol	Chain	Length	Quality of chain
3	Q	18	
4	C	229	
4	G	229	
5	D	259	
5	H	259	
6	I	2	
6	J	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	NAG	E	300	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13028 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called MHC CLASS II H2-IAg7 ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	184	Total	C	N	O	S	0	0	0
			1481	956	240	283	2			
1	E	184	Total	C	N	O	S	0	0	0
			1481	956	240	283	2			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	179	SER	-	expression tag	UNP P04228
A	180	SER	-	expression tag	UNP P04228
A	181	ALA	-	expression tag	UNP P04228
A	182	ASP	-	expression tag	UNP P04228
A	183	LEU	-	expression tag	UNP P04228
A	184	VAL	-	expression tag	UNP P04228
A	185	PRO	-	expression tag	UNP P04228
A	186	ARG	-	expression tag	UNP P04228
E	179	SER	-	expression tag	UNP P04228
E	180	SER	-	expression tag	UNP P04228
E	181	ALA	-	expression tag	UNP P04228
E	182	ASP	-	expression tag	UNP P04228
E	183	LEU	-	expression tag	UNP P04228
E	184	VAL	-	expression tag	UNP P04228
E	185	PRO	-	expression tag	UNP P04228
E	186	ARG	-	expression tag	UNP P04228

- Molecule 2 is a protein called MHC CLASS II H2-IAg7 BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	178	Total	C	N	O	S	0	0	0
			1487	934	269	278	6			
2	F	178	Total	C	N	O	S	0	0	0
			1487	934	269	278	6			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	GLY	-	expression tag	UNP Q31135
B	-4	SER	-	expression tag	UNP Q31135
B	-3	GLY	-	expression tag	UNP Q31135
B	-2	SER	-	expression tag	UNP Q31135
B	-1	GLY	-	expression tag	UNP Q31135
B	0	SER	-	expression tag	UNP Q31135
B	189	SER	-	expression tag	UNP Q31135
B	190	SER	-	expression tag	UNP Q31135
B	191	ALA	-	expression tag	UNP Q31135
B	192	ASP	-	expression tag	UNP Q31135
B	193	LEU	-	expression tag	UNP Q31135
B	194	VAL	-	expression tag	UNP Q31135
B	195	PRO	-	expression tag	UNP Q31135
B	196	ARG	-	expression tag	UNP Q31135
F	-5	GLY	-	expression tag	UNP Q31135
F	-4	SER	-	expression tag	UNP Q31135
F	-3	GLY	-	expression tag	UNP Q31135
F	-2	SER	-	expression tag	UNP Q31135
F	-1	GLY	-	expression tag	UNP Q31135
F	0	SER	-	expression tag	UNP Q31135
F	189	SER	-	expression tag	UNP Q31135
F	190	SER	-	expression tag	UNP Q31135
F	191	ALA	-	expression tag	UNP Q31135
F	192	ASP	-	expression tag	UNP Q31135
F	193	LEU	-	expression tag	UNP Q31135
F	194	VAL	-	expression tag	UNP Q31135
F	195	PRO	-	expression tag	UNP Q31135
F	196	ARG	-	expression tag	UNP Q31135

- Molecule 3 is a protein called PEPTIDE HEL 11-27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	17	Total	C	N	O	S	0	0	0
			132	81	27	23	1			
3	Q	17	Total	C	N	O	S	0	0	0
			132	81	27	23	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	10	GLY	ALA	conflict	UNP P00698

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	10	GLY	ALA	conflict	UNP P00698

- Molecule 4 is a protein called TCR 21.3 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	192	Total	C	N	O	S	0	0	0
			1494	932	253	299	10			
4	G	192	Total	C	N	O	S	0	0	0
			1494	932	253	299	10			

- Molecule 5 is a protein called TCR 21.3 beta chain.

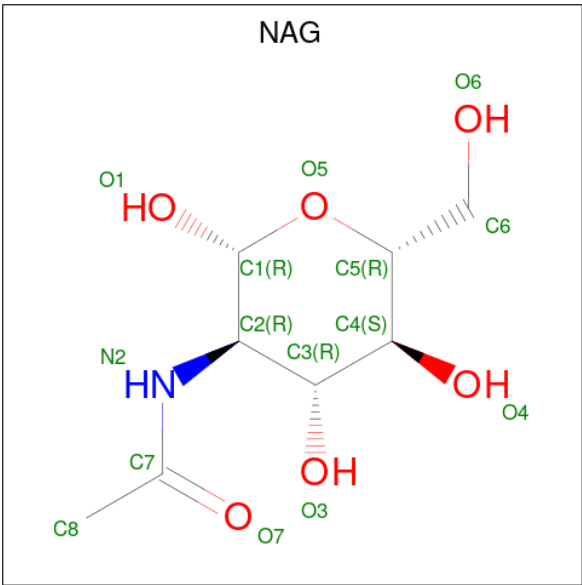
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	236	Total	C	N	O	S	0	0	0
			1878	1184	333	355	6			
5	H	236	Total	C	N	O	S	0	0	0
			1878	1184	333	355	6			

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

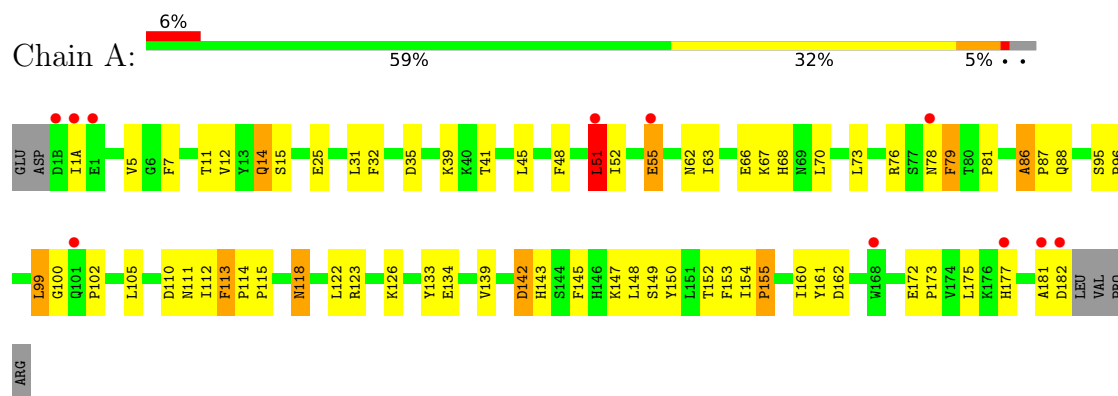


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		

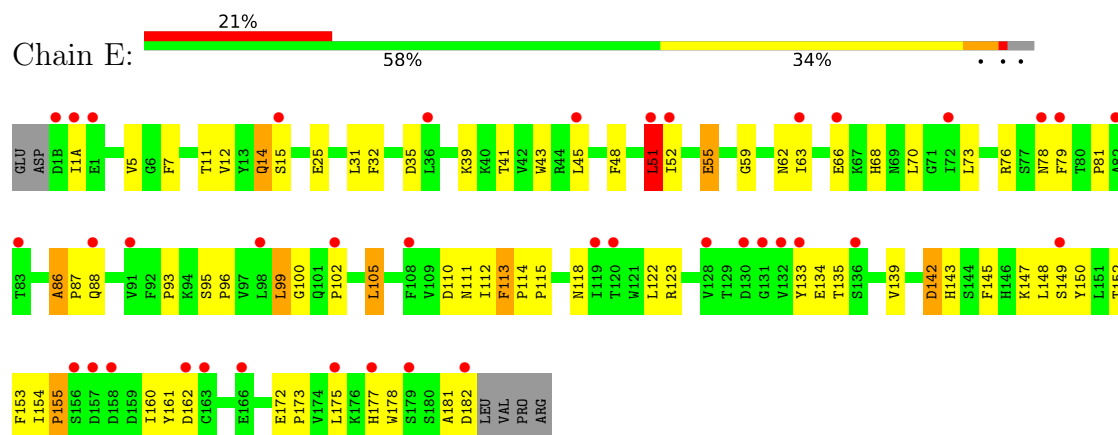
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

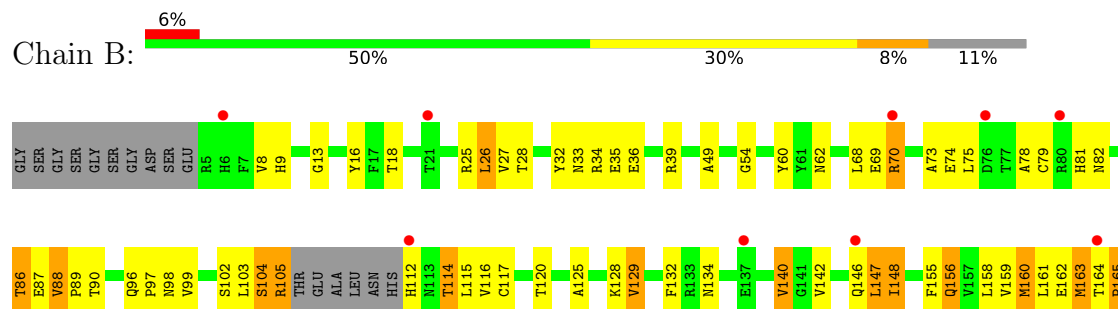
• Molecule 1: MHC CLASS II H2-IAg7 ALPHA CHAIN

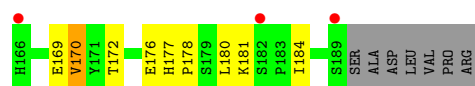


• Molecule 1: MHC CLASS II H2-IAg7 ALPHA CHAIN

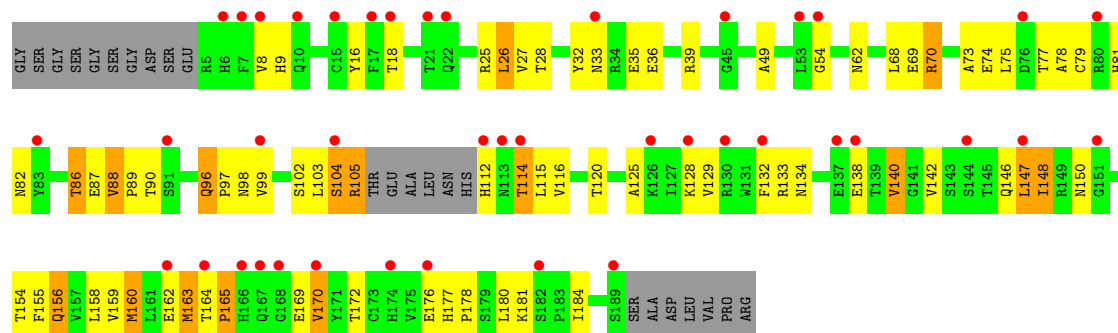


• Molecule 2: MHC CLASS II H2-IAg7 BETA CHAIN

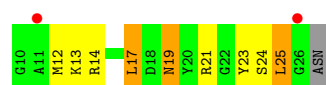
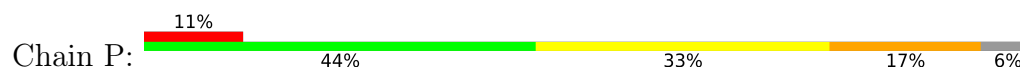




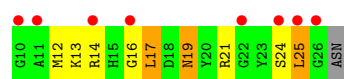
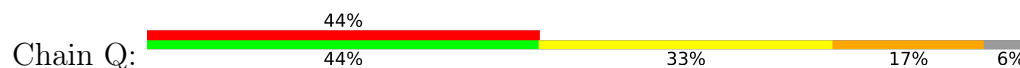
• Molecule 2: MHC CLASS II H2-IAg7 BETA CHAIN



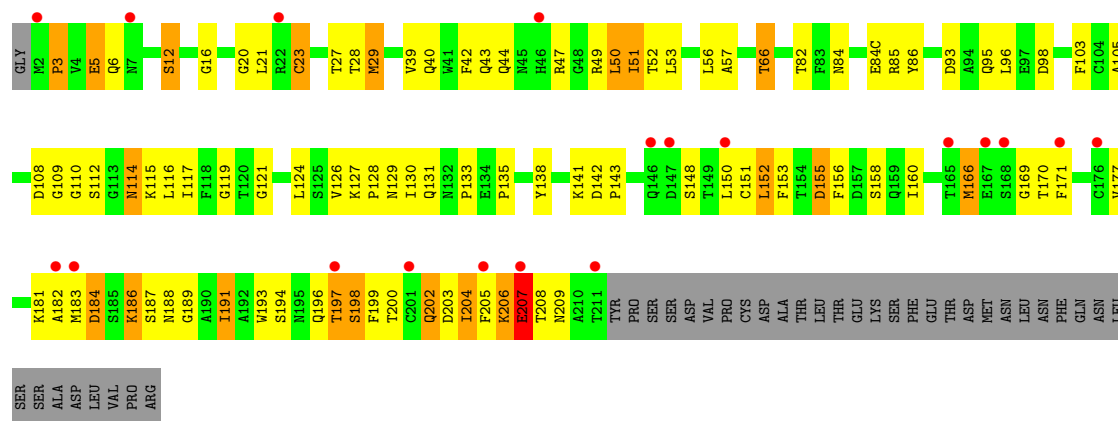
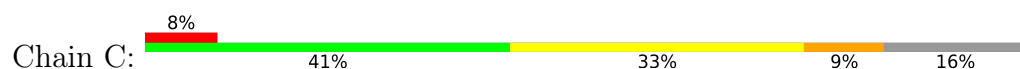
• Molecule 3: PEPTIDE HEL 11-27



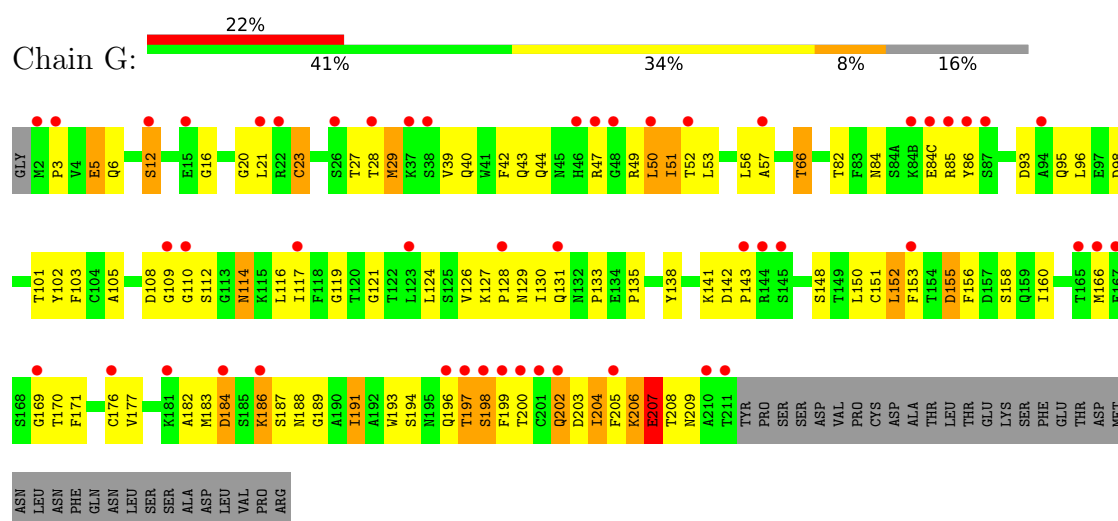
• Molecule 3: PEPTIDE HEL 11-27



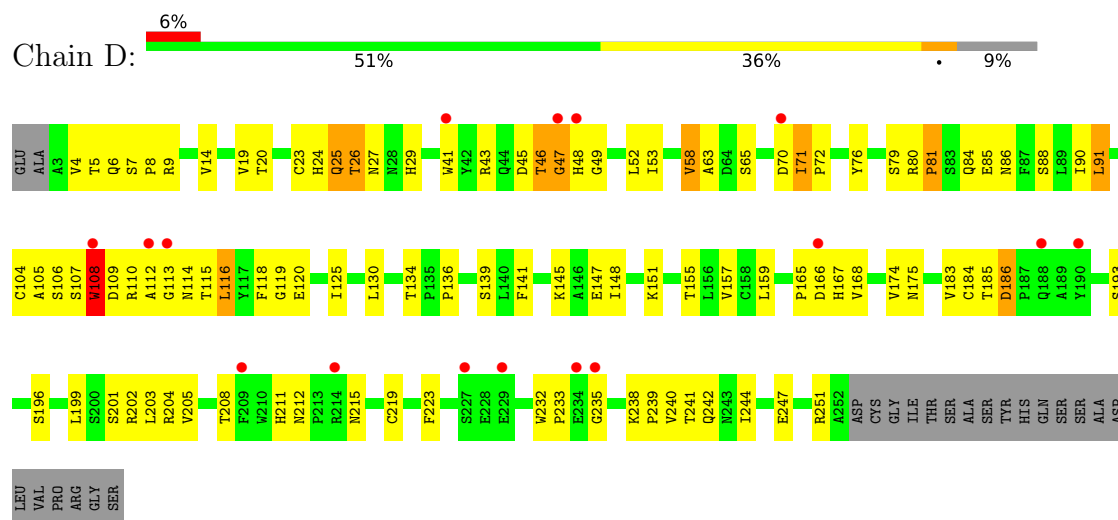
• Molecule 4: TCR 21.3 alpha chain



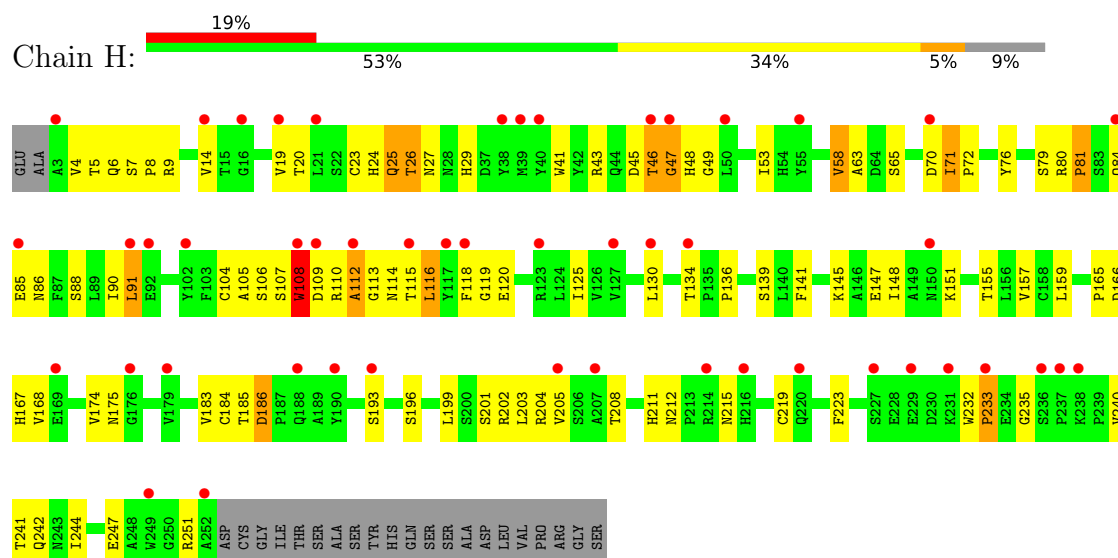
• Molecule 4: TCR 21.3 alpha chain



• Molecule 5: TCR 21.3 beta chain



• Molecule 5: TCR 21.3 beta chain



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  50% 50%

MAG1
MAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.47Å 99.39Å 404.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.26 – 2.89 48.26 – 2.89	Depositor EDS
% Data completeness (in resolution range)	54.7 (48.26-2.89) 54.7 (48.26-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.5_2	Depositor
R, R_{free}	0.253 , 0.281 0.249 , 0.277	Depositor DCC
R_{free} test set	727 reflections (2.12%)	wwPDB-VP
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	13028	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	0/1526	0.92	7/2083 (0.3%)
1	E	0.39	0/1526	0.89	6/2083 (0.3%)
2	B	0.52	0/1523	0.85	2/2064 (0.1%)
2	F	0.43	0/1523	0.82	3/2064 (0.1%)
3	P	0.38	0/134	0.71	0/176
3	Q	0.33	0/134	0.70	0/176
4	C	0.42	0/1523	0.84	0/2058
4	G	0.40	0/1523	0.83	1/2058 (0.0%)
5	D	0.52	0/1932	0.85	3/2627 (0.1%)
5	H	0.41	0/1932	0.82	1/2627 (0.0%)
All	All	0.45	0/13276	0.85	23/18016 (0.1%)

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	ALA	CA-C-N	8.40	129.07	119.99
1	A	86	ALA	C-N-CA	8.40	129.07	119.99
1	E	86	ALA	CA-C-N	8.14	128.78	119.99
1	E	86	ALA	C-N-CA	8.14	128.78	119.99
1	A	172	GLU	CA-C-N	5.56	126.80	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1481	0	1412	56	0
1	E	1481	0	1412	60	0
2	B	1487	0	1422	63	0
2	F	1487	0	1422	57	0
3	P	132	0	126	9	0
3	Q	132	0	126	8	0
4	C	1494	0	1443	83	0
4	G	1494	0	1443	82	0
5	D	1878	0	1785	66	0
5	H	1878	0	1785	69	0
6	I	28	0	25	1	0
6	J	28	0	25	0	0
7	A	14	0	13	1	0
7	E	14	0	13	0	0
All	All	13028	0	12452	500	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

The worst 5 of 500 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:136:PRO:HD2	5:H:244:ILE:HD12	1.49	0.95
5:H:193:SER:HB2	5:H:196:SER:HB3	1.48	0.95
5:D:136:PRO:HD2	5:D:244:ILE:HD12	1.50	0.94
5:D:193:SER:HB2	5:D:196:SER:HB3	1.50	0.93
1:A:115:PRO:HG3	1:A:145:PHE:CE1	2.04	0.93

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	182/190 (96%)	154 (85%)	22 (12%)	6 (3%)	3	11
1	E	182/190 (96%)	155 (85%)	22 (12%)	5 (3%)	4	14
2	B	174/201 (87%)	144 (83%)	26 (15%)	4 (2%)	5	17
2	F	174/201 (87%)	144 (83%)	26 (15%)	4 (2%)	5	17
3	P	15/18 (83%)	10 (67%)	3 (20%)	2 (13%)	0	0
3	Q	15/18 (83%)	10 (67%)	3 (20%)	2 (13%)	0	0
4	C	190/229 (83%)	156 (82%)	23 (12%)	11 (6%)	1	3
4	G	190/229 (83%)	157 (83%)	23 (12%)	10 (5%)	1	4
5	D	234/259 (90%)	208 (89%)	18 (8%)	8 (3%)	3	11
5	H	234/259 (90%)	207 (88%)	19 (8%)	8 (3%)	3	11
All	All	1590/1794 (89%)	1345 (85%)	185 (12%)	60 (4%)	2	9

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	A	113	PHE
2	B	104	SER
3	P	17	LEU
4	C	182	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	165/171 (96%)	151 (92%)	14 (8%)	10	28
1	E	165/171 (96%)	151 (92%)	14 (8%)	10	28
2	B	164/181 (91%)	148 (90%)	16 (10%)	7	22
2	F	164/181 (91%)	148 (90%)	16 (10%)	7	22
3	P	12/13 (92%)	10 (83%)	2 (17%)	2	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Q	12/13 (92%)	10 (83%)	2 (17%)	2	6
4	C	168/202 (83%)	149 (89%)	19 (11%)	5	17
4	G	168/202 (83%)	148 (88%)	20 (12%)	5	15
5	D	204/222 (92%)	182 (89%)	22 (11%)	6	19
5	H	204/222 (92%)	182 (89%)	22 (11%)	6	19
All	All	1426/1578 (90%)	1279 (90%)	147 (10%)	7	21

5 of 147 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	G	166	MET
5	H	208	THR
4	G	191	ILE
5	H	58	VAL
4	C	203	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	64	GLN
4	G	188	ASN
2	F	81	HIS
4	G	46	HIS
5	H	25	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

4 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	I	1	6,5	14,14,15	0.77	1 (7%)	17,19,21	1.45	2 (11%)
6	NAG	I	2	6	14,14,15	0.58	0	17,19,21	1.23	1 (5%)
6	NAG	J	1	6,5	14,14,15	0.76	1 (7%)	17,19,21	1.46	2 (11%)
6	NAG	J	2	6	14,14,15	0.62	0	17,19,21	1.23	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	I	1	6,5	-	2/6/23/26	0/1/1/1
6	NAG	I	2	6	-	0/6/23/26	0/1/1/1
6	NAG	J	1	6,5	-	2/6/23/26	0/1/1/1
6	NAG	J	2	6	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	1	NAG	O5-C1	-2.23	1.39	1.43
6	J	1	NAG	O5-C1	-2.05	1.40	1.43

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	1	NAG	C1-O5-C5	3.97	117.51	112.19
6	J	1	NAG	C4-C3-C2	3.74	116.50	111.02
6	J	1	NAG	C1-O5-C5	3.48	116.85	112.19
6	I	2	NAG	C1-O5-C5	3.46	116.82	112.19
6	I	1	NAG	C4-C3-C2	3.38	115.97	111.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

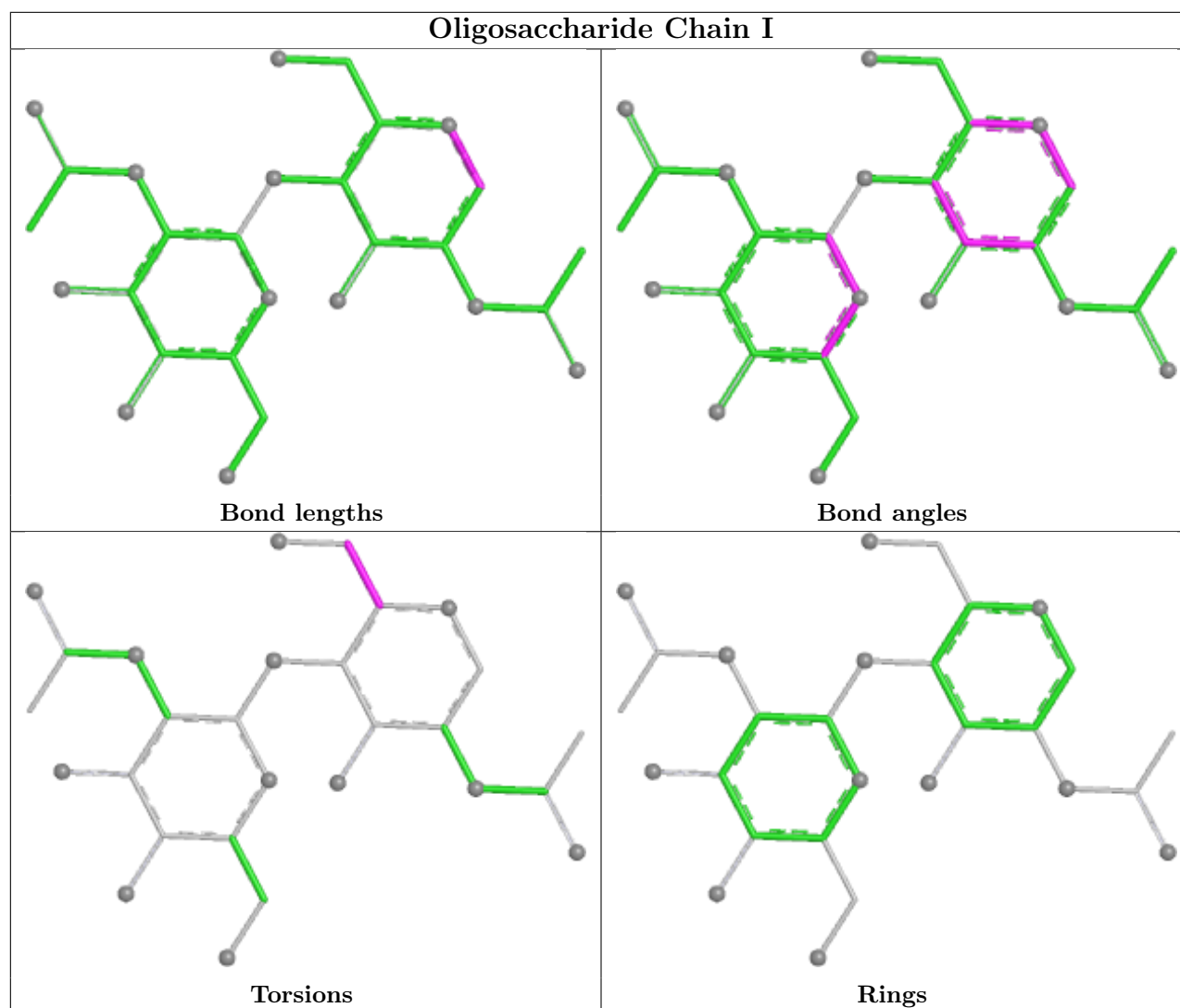
Mol	Chain	Res	Type	Atoms
6	I	1	NAG	O5-C5-C6-O6
6	J	1	NAG	O5-C5-C6-O6
6	I	1	NAG	C4-C5-C6-O6
6	J	1	NAG	C4-C5-C6-O6

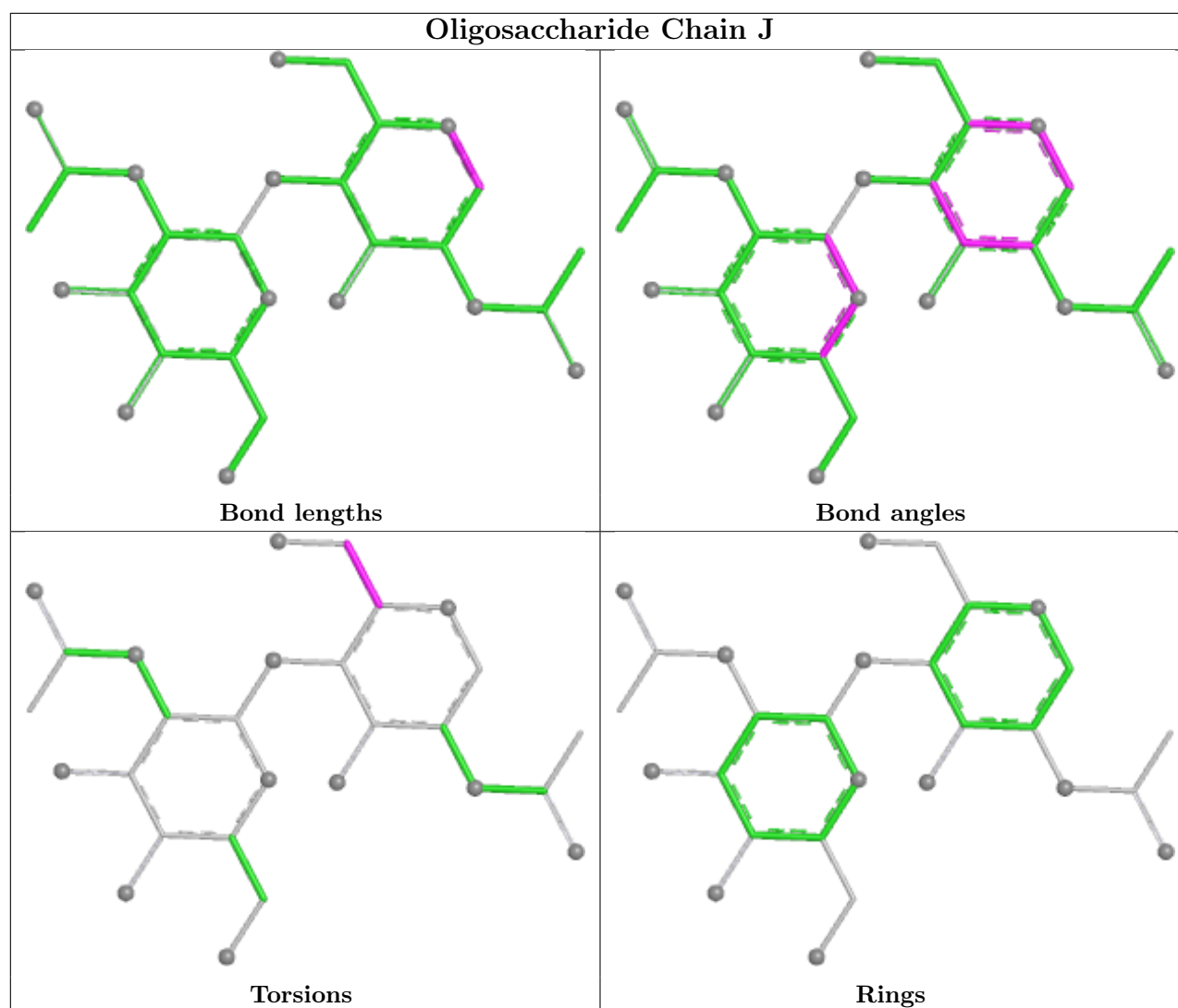
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	A	300	1	14,14,15	0.47	0	17,19,21	0.92	0
7	NAG	E	300	1	14,14,15	0.52	0	17,19,21	0.94	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	300	1	-	5/6/23/26	0/1/1/1
7	NAG	E	300	1	1/1/5/7	5/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	300	NAG	C1-O5-C5	2.04	114.91	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	E	300	NAG	C1

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	300	NAG	C3-C2-N2-C7
7	A	300	NAG	C8-C7-N2-C2
7	A	300	NAG	O7-C7-N2-C2
7	E	300	NAG	C3-C2-N2-C7
7	E	300	NAG	C8-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	300	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	184/190 (96%)	0.41	11 (5%)	27 21	15, 39, 92, 151	0
1	E	184/190 (96%)	1.35	39 (21%)	2 2	48, 93, 146, 164	0
2	B	178/201 (88%)	0.51	12 (6%)	24 19	16, 51, 104, 149	0
2	F	178/201 (88%)	1.35	41 (23%)	2 2	43, 91, 153, 192	0
3	P	17/18 (94%)	0.91	2 (11%)	9 8	14, 30, 89, 90	0
3	Q	17/18 (94%)	2.12	8 (47%)	0 0	51, 83, 139, 144	0
4	C	192/229 (83%)	0.85	19 (9%)	13 11	13, 60, 125, 156	0
4	G	192/229 (83%)	1.32	50 (26%)	1 1	45, 84, 136, 169	0
5	D	236/259 (91%)	0.35	16 (6%)	23 18	9, 37, 86, 139	0
5	H	236/259 (91%)	1.32	49 (20%)	2 2	50, 84, 135, 166	0
All	All	1614/1794 (89%)	0.94	247 (15%)	5 4	9, 69, 133, 192	0

The worst 5 of 247 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1(A)	ILE	6.8
2	F	138	GLU	5.8
5	D	112	ALA	5.8
2	F	189	SER	5.4
2	B	189	SER	5.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

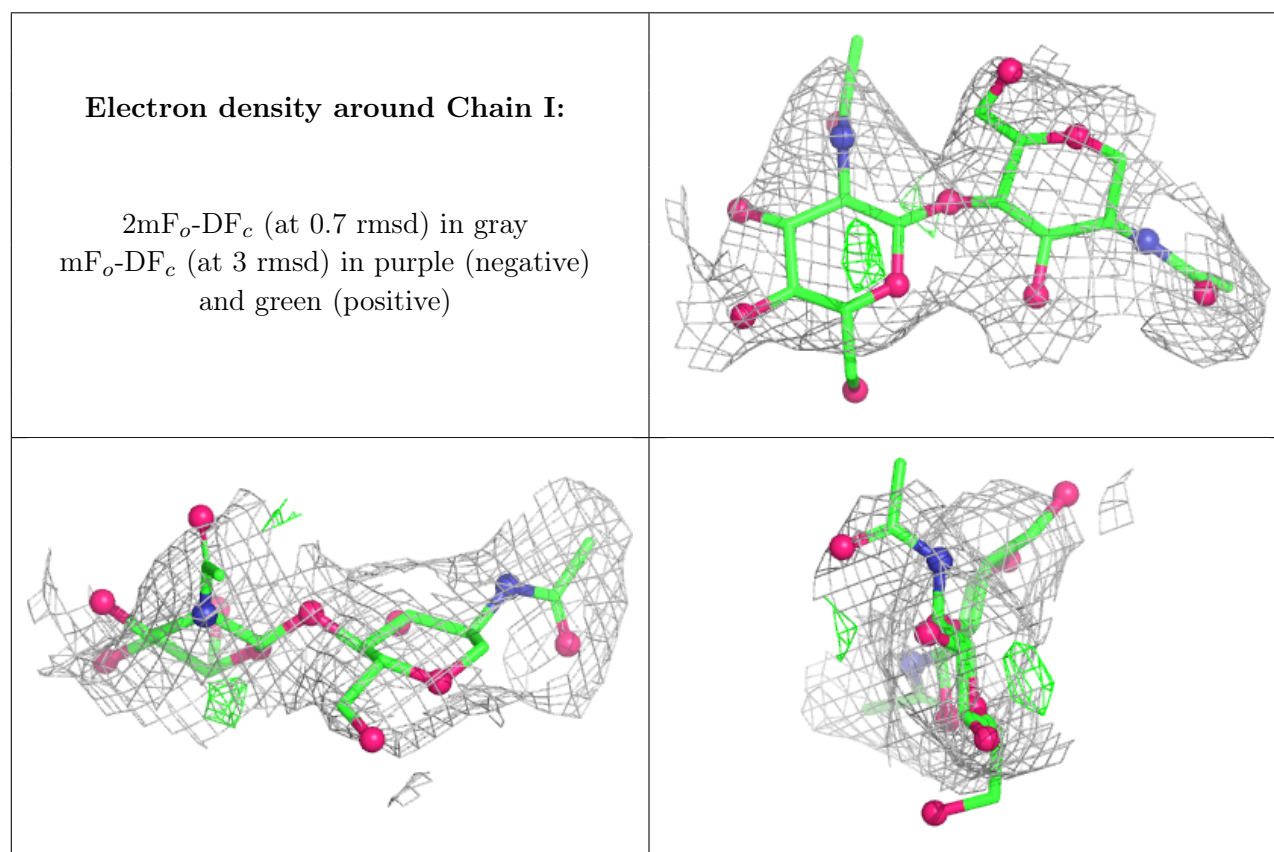
There are no non-standard protein/DNA/RNA residues in this entry.

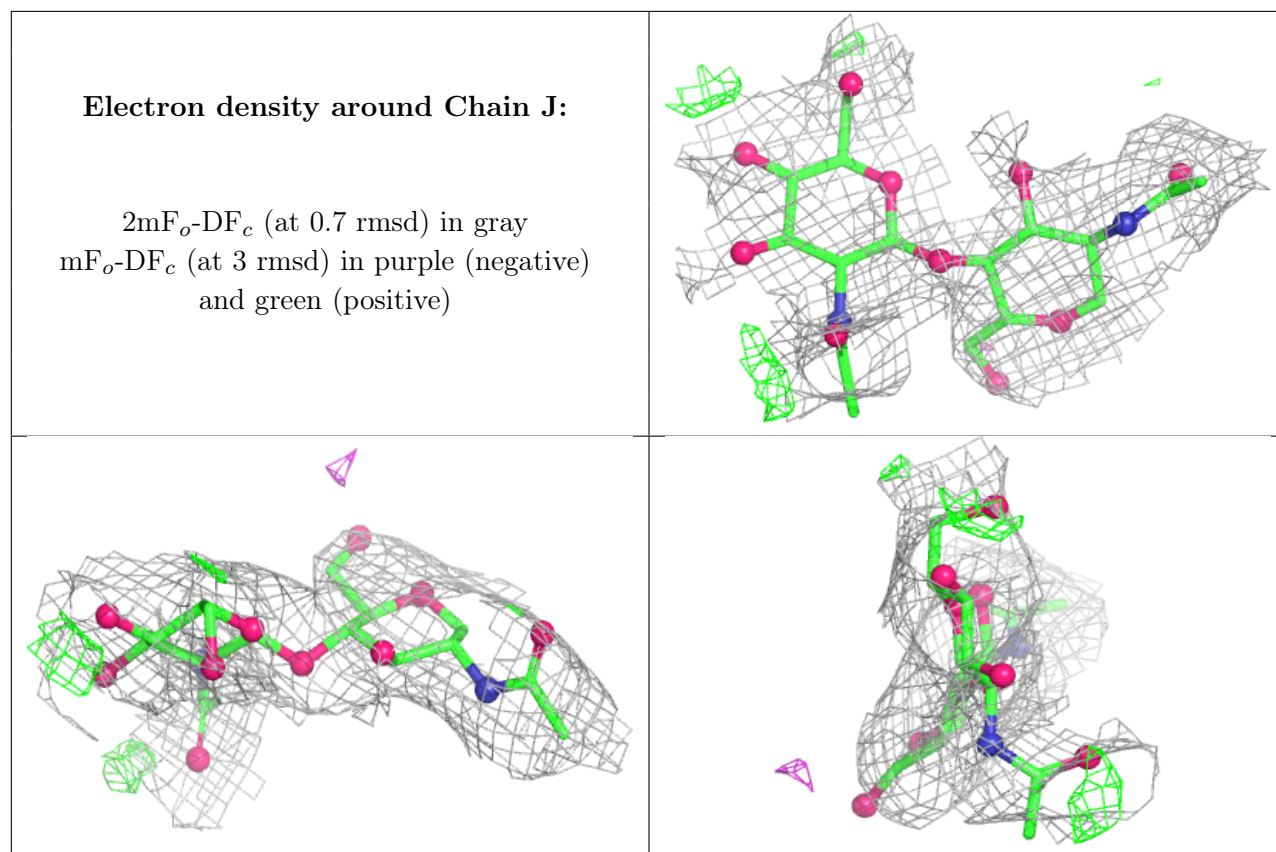
6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	I	1	14/15	-	-	39,41,42,43	0
6	NAG	I	2	14/15	-	-	122,123,125,126	0
6	NAG	J	1	14/15	-	-	71,73,74,75	0
6	NAG	J	2	14/15	-	-	128,130,132,132	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	E	300	14/15	0.53	0.19	169,171,172,173	0
7	NAG	A	300	14/15	0.62	0.26	119,121,122,123	0

6.5 Other polymers [i](#)

There are no such residues in this entry.